

Toyota Research Institute Brings Artificial Intelligence to the Hunt for New Materials

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Palo Alto, Calif., March 30, 2017 — The Toyota Research Institute (TRI) will collaborate with research entities, universities and companies on materials science research, investing approximately \$35 million over the next four years in research that uses artificial intelligence to help accelerate the design and discovery of advanced materials. Initially, the program will aim to help revolutionize materials science and identify new advanced battery materials and fuel cell catalysts that can power future zero-emissions and carbon-neutral vehicles.

“Toyota recognizes that artificial intelligence is a vital basic technology that can be leveraged across a range of industries, and we are proud to use it to expand the boundaries of materials science,” said TRI Chief Science Officer Eric Krotkov. “Accelerating the pace of materials discovery will help lay the groundwork for the future of clean energy and bring us even closer to achieving Toyota’s vision of reducing global average new-vehicle CO2 emissions by 90 percent by 2050.”

Initial research projects include collaborations with Stanford University, the Massachusetts Institute of Technology, the University of Michigan, the University at Buffalo, the University of Connecticut, , and the U.K.-based materials science company Ilika. TRI is also in ongoing discussions with additional research partners.

“This represents a fantastic opportunity to drastically advance the use of databases and machine learning methods in materials discovery,” said Jens Norskov, Professor at Stanford University and director of the SUNCAT center. “The partnership combines theory, computation and experiment in an unprecedented, concerted effort. We are particularly excited by prospects for an avant-garde approach to catalyst development for fuel cells.”

Research will merge advanced computational materials modeling, new sources of experimental data, machine learning and artificial intelligence in an effort to reduce the time scale for new materials development from a period that has historically been measured in decades. Research programs will follow parallel paths, working to identify new materials for use in future energy systems as well as to develop tools and processes that can accelerate the design and development of new materials more broadly.

In support of these goals, TRI will partner on projects focused on areas including:

- The development of new models and materials for batteries and fuel cells;
- Broader programs to pursue novel uses of machine learning, artificial intelligence and materials informatics approaches for the design and development new materials; and,
- New automated materials discovery systems that integrate simulation, machine learning, artificial intelligence and/or robotics.

Accelerating materials science discovery represents one of four core focus areas for TRI, which was launched in 2015 with mandates to also enhance auto safety with automated technologies, increase access to mobility for

those who otherwise cannot drive and help translate outdoor mobility technology into products for indoor mobility.